

Universität Freiburg
Advanced physics lab , part 1
Holiday internship in the summer semester 2024

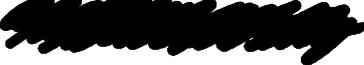
Experiment 4

I^2 molecule


(Group 11)

November 5, 2024

Dates of experimental execution: September 10th to 11th, 2024

Tutor: 

Contents

1	Goal of the experiment	1
2	Experiment	1
2.1	Setup	1
2.2	Execution	2
3	Evaluation and error analysis	2
3.1	Calibration of the grating spectrometer	2
3.2	Absorption spectrum of iodine	2
3.3	Emission spectrum of iodine	6
4	Discussion	9
4.1	Final results	9
4.2	Comparison with expected results	9
4.2.1	Absorption spectrum of iodine	9
4.2.2	Emission spectrum of iodine	10
4.3	Improvements and Suggestions	11
5	Attachment	12
5.1	Lab book	12
	literature	13

1 Goal of the experiment

The goal of this experiment is to measure the absorption and emission spectrum of the iodine molecule and determine the characteristics of the diatomic iodine molecule.

2 Experiment

2.1 Setup

For this experiment multiple setups were used depending on the desired measurement. For the calibration of the spectrometer a mercury-vapor-lamp is used and a sodium-vapor-lamp to control it. The setup is shown in [figure 1](#). For this setup 2 lenses and mirrors were used to focus the beam on the tube with the iodine gas. The tube had a heating system. Behind the tube is an aperture and the grating spectrometer.

For the measurement of the absorption spectrum a halogen lamp and a LED have been used as shown in the lab book [figure 11](#) in the attachments. For some measurements the halogen lamp was used without an aperture.

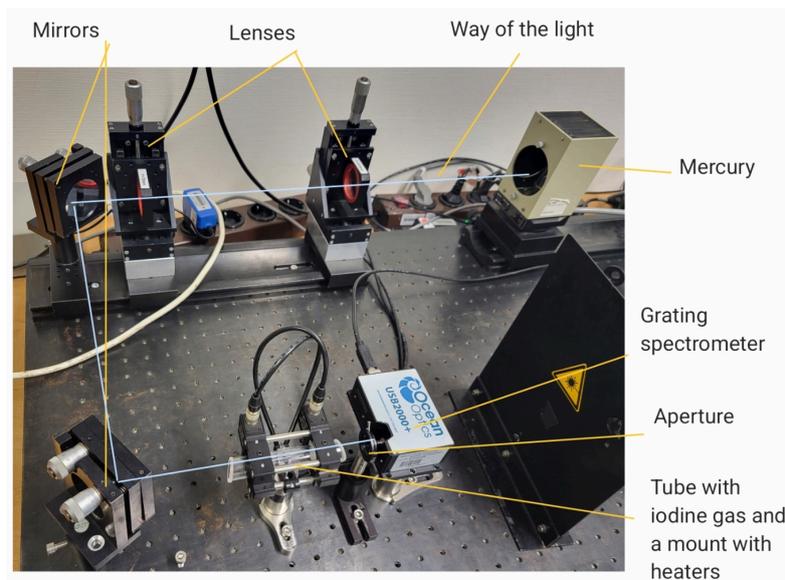


Figure 1: Setup for the calibration spectrum measurement

For the measurement of the emission spectrum a laser and a mirror were used as shown in [figure 2](#). In addition the Laser had a heating system.

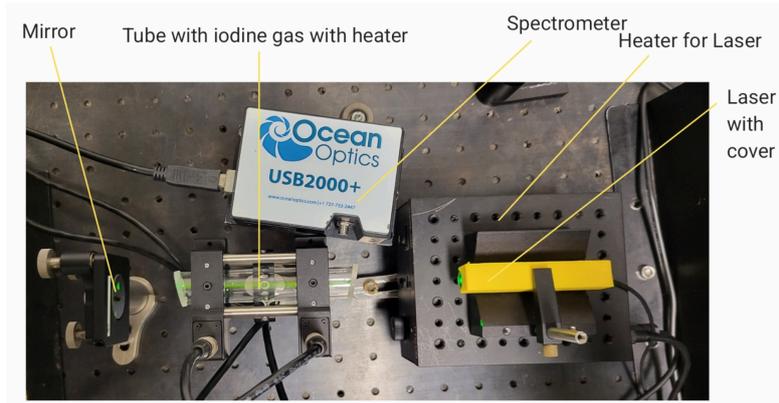


Figure 2: Setup for the emission spectrum measurement

2.2 Execution

First the spectrometer was calibrated with the known Hg-spectrum. The light intensity in the spectrometer was controlled with the aperture. The calibration was done in the spectrometer software on the computer. For the measurements the iodine was heated for the calibration and the absorption spectrum. For the emission measurement the laser was heated but the iodine gas was not.

3 Evaluation and error analysis

3.1 Calibration of the grating spectrometer

The calibration of the spectrometer was done as said by the user manual[1]. The tube with the I^2 -gas was heated to $T_T = 65^\circ\text{C}$. After the calibration the spectral lines of mercury and sodium matched with their literature values with an value $\pm a = 1\text{ nm}$. This is considered triangularly distributed. Therefore the uncertainty on the wavelength is $\Delta\lambda = \frac{1\text{ nm}}{\sqrt{6}} \approx 0.4\text{ nm}$. Later, this value is used as the uncertainty on the measured wavelength. All the uncertainties come from the errors of the used values through the Gaussian error propagation

$$\Delta A = \sqrt{\left(\frac{\partial A}{\partial x} \cdot \Delta x\right)^2 + \left(\frac{\partial A}{\partial y} \cdot \Delta y\right)^2}.$$

3.2 Absorption spectrum of iodine

The iodine-tube was heated again to $T_T = 65^\circ\text{C}$. The best result was achieved with a halogen lamp far away from the tube with the spectrometer right behind it. An aperture

was not used. The absorption occurs from the singlet ground state to the first excited triplet state



These states between which the transition happens are illustrated in [figure 3](#) with their vibrational levels.

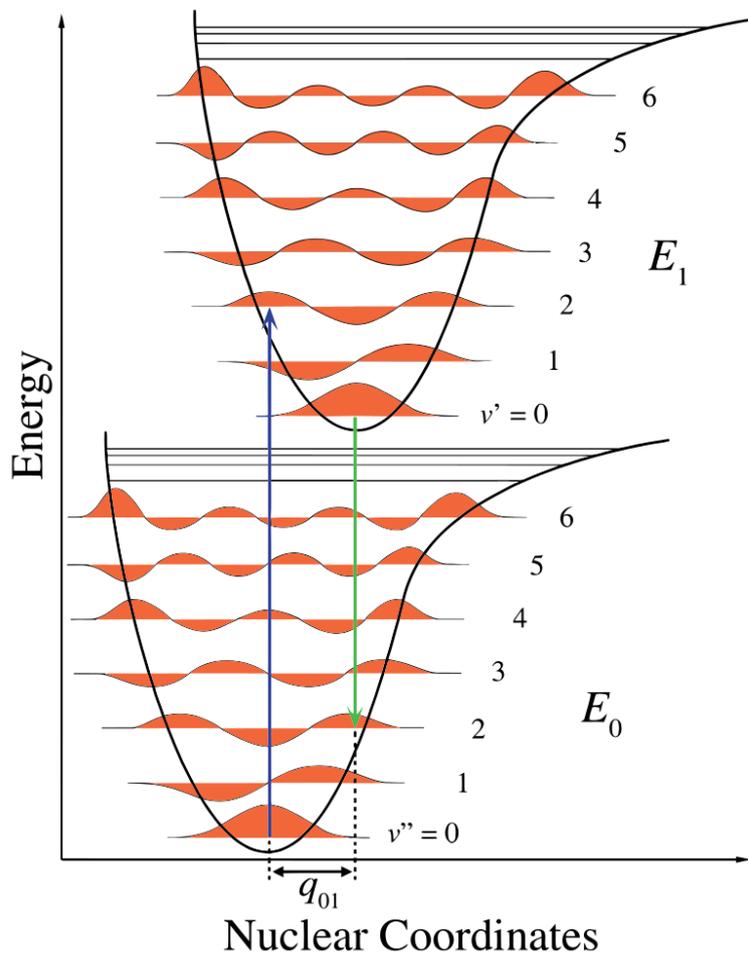


Figure 3: Diagram of the Franck-Condon principle energy[2]

The absorption spectrum in [figure 4](#) is achieved by subtracting the signals coming from the the halogen lamp without the iodine from the total signals.

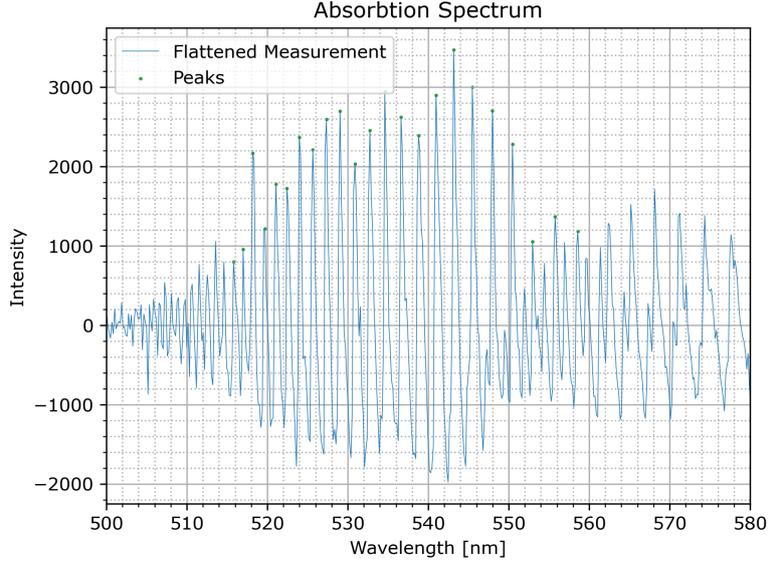


Figure 4: Absorption spectrum of iodine

In the ground state the lowest vibration level is relevant $v'' = 0$. From there the I^2 molecules are excited to different v' vibration levels and absorb light in the process. The transition $v'' = 0 \rightarrow v' = 25$ is known to happen at $\lambda_{v''=0 \rightarrow v'=25 \text{ nm}} = 545.8 \text{ nm}$. With that reference the other absorbance peaks can be assigned to specific transitions. For the analysis the wavelengths are converted into wave numbers $\tilde{\nu}$. They are calculated with $\tilde{\nu} = 1/\lambda$.

The Morse potential is a model of the vibrational structure of diatomic molecules. It is defined by the [equation \(2\)](#) with

$$V(r) = D_e \left(1 - e^{-\beta(r-r_0)}\right)^2 \quad (2)$$

with the Morse parameter $\beta = \sqrt{k/2D_e}$ and the equilibrium bond distance r_0 . From the Morse potential the equation for the vibration levels [equation \(3\)](#) can be found.

$$G_v = \omega_0 \left(v + \frac{1}{2}\right) - \omega_0 x_0 \left(v + \frac{1}{2}\right)^2 \quad (3)$$

There, ω_0 is the fundamental frequency and $\omega_0 x_0$ is the anharmonicity. In [equation \(4\)](#)[\[3\]](#) ω_0 is calculated by

$$\omega_0 = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}} = \frac{\beta}{c} \sqrt{\frac{D_e}{2\pi^2 \mu}}. \quad (4)$$

The reduced mass of the I^2 molecule is calculated with the atomic mass $A = (126.904 47 \pm 0.000 03) \text{ u}$ [\[4\]](#) and the Gaussian error propagation to $\mu = (1.053 65 \pm 0.000 03) \times 10^{-25} \text{ kg}$.

The dissociation energy D_e is calculated with the Birge-Sponer method by

$$D_e = \sum_{v=0}^{v_{\max}} \Delta G_{v+\frac{1}{2}} = G(v_{\max} + 1) - G(0) = \frac{\omega_0^2}{4\omega_0 x_0}. \quad (5)$$

Finally in the Birge-Sponer plot [figure 5](#) the energy difference to the next vibration level is shown and fitted with

$$\Delta G_v = \omega_0 - 2\omega_0 x_0(v + 1). \quad (6)$$

The y-axis intercept is the frequency

$$\omega_0 = (134 \pm 2) \text{ cm}^{-1}$$

of the iodine. Half of the slopes value is the anharmonicity

$$\omega_0 x_0 = (1.06 \pm 0.02) \text{ cm}^{-1}$$

and the dissociation energy

$$D_e = (0.53 \pm 0.01) \text{ eV}$$

can be calculated with [equation \(5\)](#)

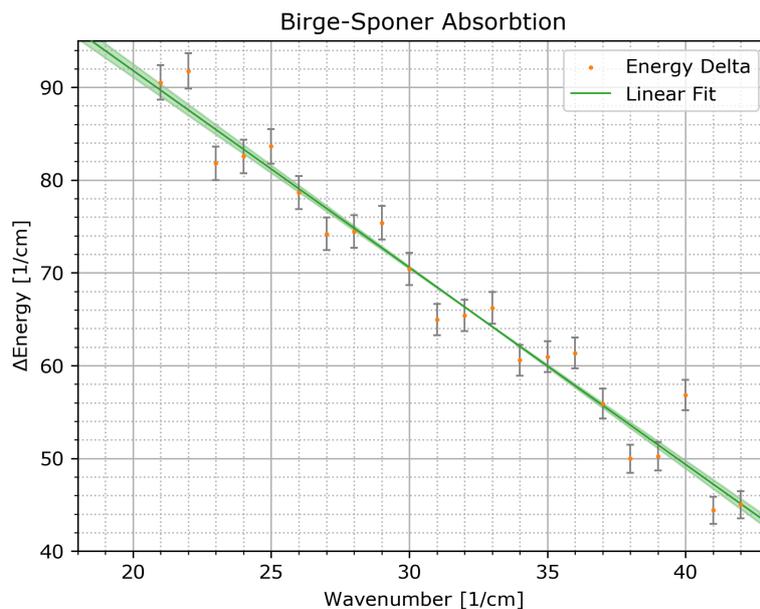


Figure 5: Birge-Sponer plot for the $v'' = 0 \rightarrow v'$ absorption

In [figure 6](#) the resulting Morse potential of the emission spectrum is illustrated in blue compared to the literature value in orange.

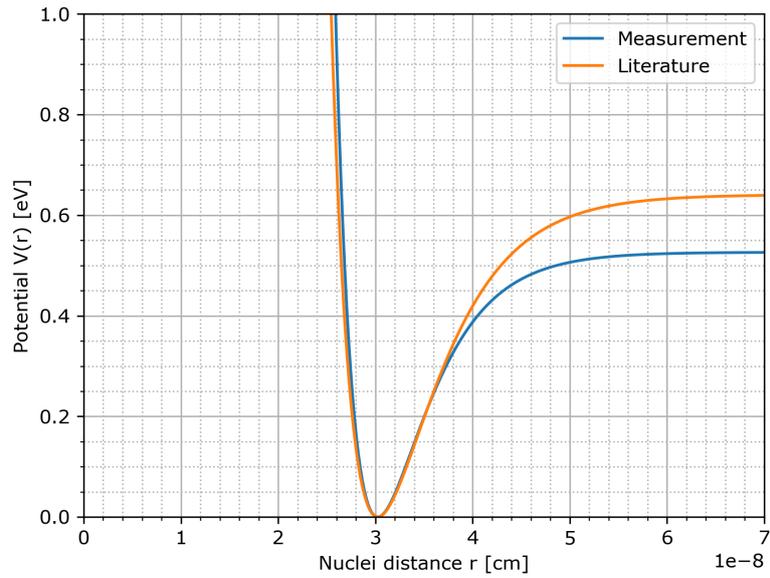


Figure 6: Morse potential for the absorption

3.3 Emission spectrum of iodine

For this measurement a thorlabs laser with the wavelength $\lambda = 532 \text{ nm}$ ^[5] was used. the iodine is at room temperature and the laser is heated to $T_L = 25.0 \text{ celsius}$. With these settings of the laser a bright light beam (figure 7) with a warmer color then the laser light could be seen in the tube.

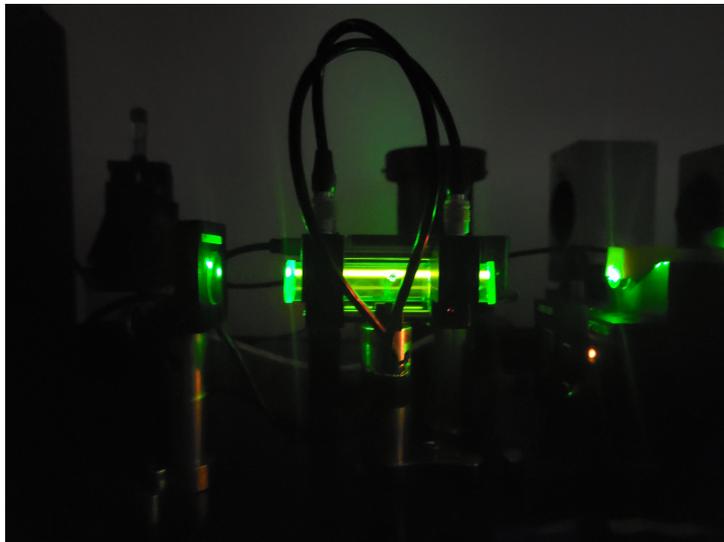


Figure 7: Laser induced emission of iodine

For the emission electrons fall back from the excited state to the ground state. The $\lambda = 532$ nm laser induces the transmission from the $v' = 32$ excited B state back to the v'' vibrational X ground states[3]. Depending on the hit v'' state a different amount of energy is set free and therefore light with a certain wavelength is emitted. The detected wavelengths are illustrated in figure 8. The laser peak is cut of and is in parts visible at the left side of the plot. In the plot is the intensity of the peaks with certain wavelengths visible.

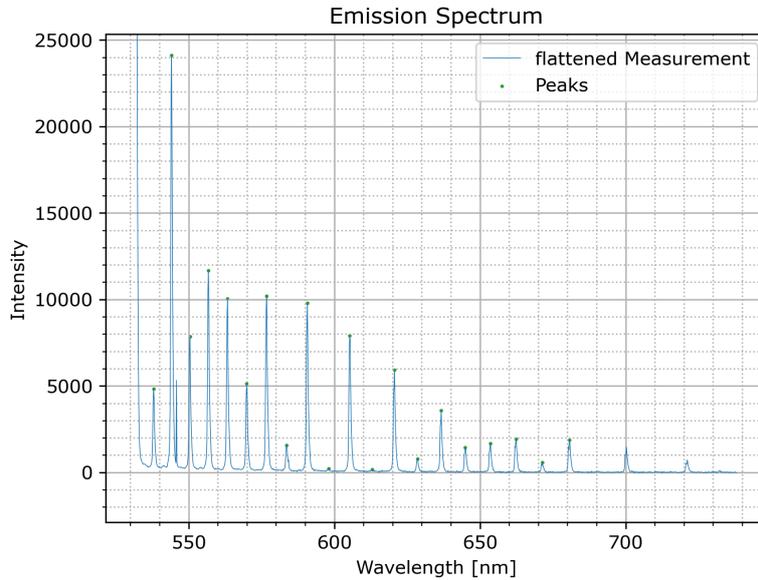


Figure 8: Emission spectrum of iodine

In the same way to the absorbance section the Birge-Sponer plot in figure 9 is made for the $v' = 32 \rightarrow v''$ emission. The measured values are plotted with their error bars. A linear fit with equation (6) was made with an uncertainty band.

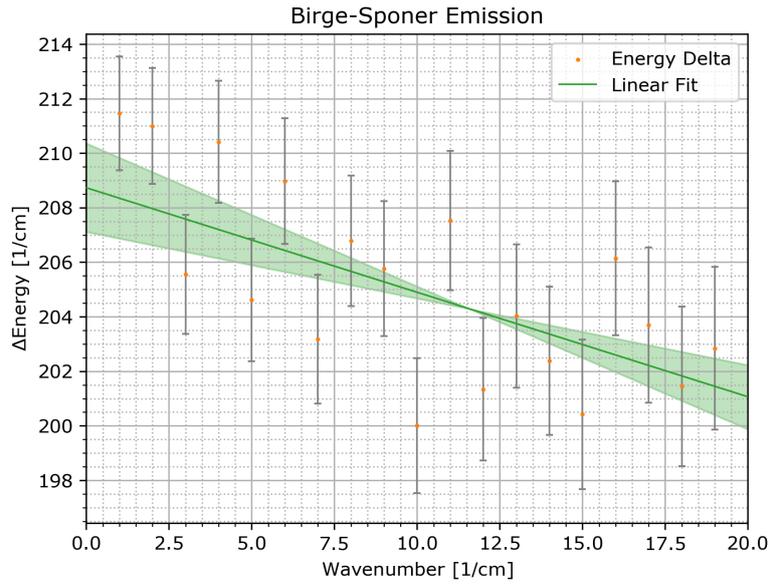


Figure 9: Birge-Sponer plot for the $v' = 32 \rightarrow v''$ emission

The y-axis intercept is again the frequency

$$\omega_0 = (208 \pm 2) \text{ cm}^{-1}$$

of the iodine. Half of the slopes value is the anharmonicity

$$\omega_0 x_0 = (0.19 \pm 0.07) \text{ cm}^{-1}$$

and the dissociation energy is

$$D_e = (7 \pm 3) \text{ eV}.$$

In [figure 10](#) the resulting Morse potential of the emission spectrum is illustrated compared to the literature value.

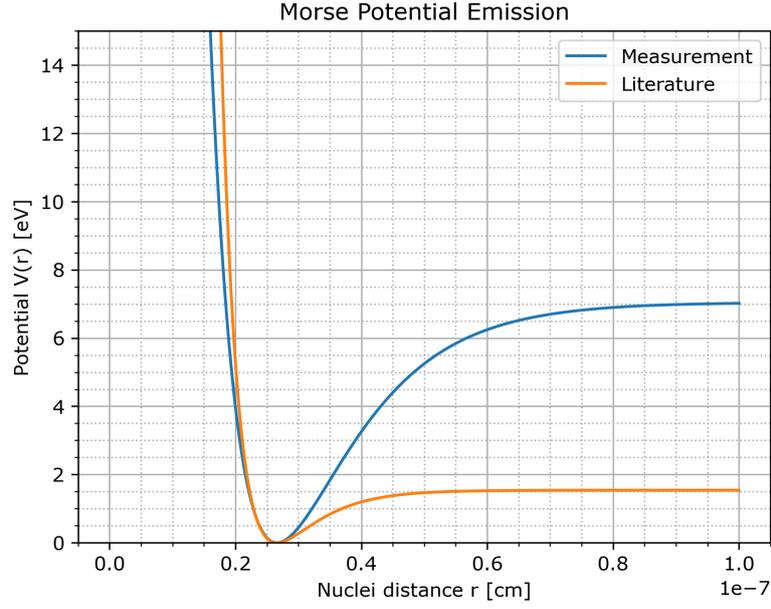


Figure 10: Morse Potential of the emission

4 Discussion

4.1 Final results

The values for the absorption spectrum are

$$\begin{aligned}\omega_0 &= (134 \pm 2) \text{ cm}^{-1}, \\ \omega_0 x_0 &= (1.06 \pm 0.02) \text{ cm}^{-1}, \\ D_e &= (0.53 \pm 0.01) \text{ eV}.\end{aligned}$$

The values for the emission spectrum are

$$\begin{aligned}\omega_0 &= (208 \pm 2) \text{ cm}^{-1}, \\ \omega_0 x_0 &= (0.19 \pm 0.07) \text{ cm}^{-1}, \\ D_e &= (7 \pm 3) \text{ eV}.\end{aligned}$$

4.2 Comparison with expected results

4.2.1 Absorption spectrum of iodine

The literature values[6] of the $v' = 32 \rightarrow$ emission spectrum are for the fundamental frequency

$$\omega_0 = 125.69 \text{ cm}^{-1}, \quad (7)$$

for the anharmonicity

$$\omega_0 x_0 = 0.764 \text{ cm}^{-1}, \quad (8)$$

and for the dissociation energy is calculated with [equation \(5\)](#) to the value

$$D_e = 0.64 \text{ eV}. \quad (9)$$

With the t-test the measured values are compared with the literature values. For $t \geq 2$ are significantly apart from each other.

$$t = \frac{|\widehat{\omega}_0 - \omega_{0,\text{lit}}|}{\Delta\omega_0} = 4.2 > 2$$

The fundamental frequency is far apart from the literature.

$$t = \frac{|\widehat{\omega_0 x_0} - \omega_0 x_{0,\text{lit}}|}{\Delta\omega_0 x_0} = 1.5 < 2$$

The anharmonicity is tolerated compared with the literature value. So the slope of [figure 5](#) is close to the literature.

$$t = \frac{|\widehat{D}_e - D_{e,\text{lit}}|}{\Delta D_e} = 1.1 < 2$$

So the dissociation energy is compatible with the literature value.

4.2.2 Emission spectrum of iodine

The literature values[3] of the $v' = 32 \rightarrow$ emission spectrum are for the fundamental frequency

$$\omega_0 = 214 \text{ cm}^{-1}, \quad (10)$$

for the anharmonicity

$$\omega_0 x_0 = 0.67 \text{ cm}^{-1}, \quad (11)$$

and for the dissociation energy

$$D_e = 1.54 \text{ eV}. \quad (12)$$

$$t = \frac{|\widehat{\omega}_0 - \omega_{0,\text{lit}}|}{\Delta\omega_0} = 3 > 2$$

The fundamental frequency is also significantly apart from the literature.

$$t = \frac{|\widehat{\omega_0 x_0} - \omega_0 x_{0,\text{lit}}|}{\Delta\omega_0 x_0} = 6.9 > 2$$

The anharmonicity is significantly apart from the literature value. So the slope of [figure 9](#) is far away from the literature.

$$t = \frac{|\widehat{D}_e - D_{e,\text{lit}}|}{\Delta D_e} = 1.8 < 2$$

So the dissociation energy is compatible with the literature value, although the previous values were far away from the literature.

4.3 Improvements and Suggestions

All in all the peaks were quite nicely visible. The data calculated was not that fitting to the literature values. A possible reason could be, that the calibration was good in the low wavelength regime, this was tested with the Sodium lamp. This is not surprising because the Mercury lamp has many lines in this low wavelength regime. The Emission spectrum on the other hand is in the high wavelength regime and is therefore worse calibrated. This can be fixed by calibrating with another lamp with spectral lines in the high wavelength regime from ca. 550nm to 750nm.

5 Attachment

5.1 Lab book

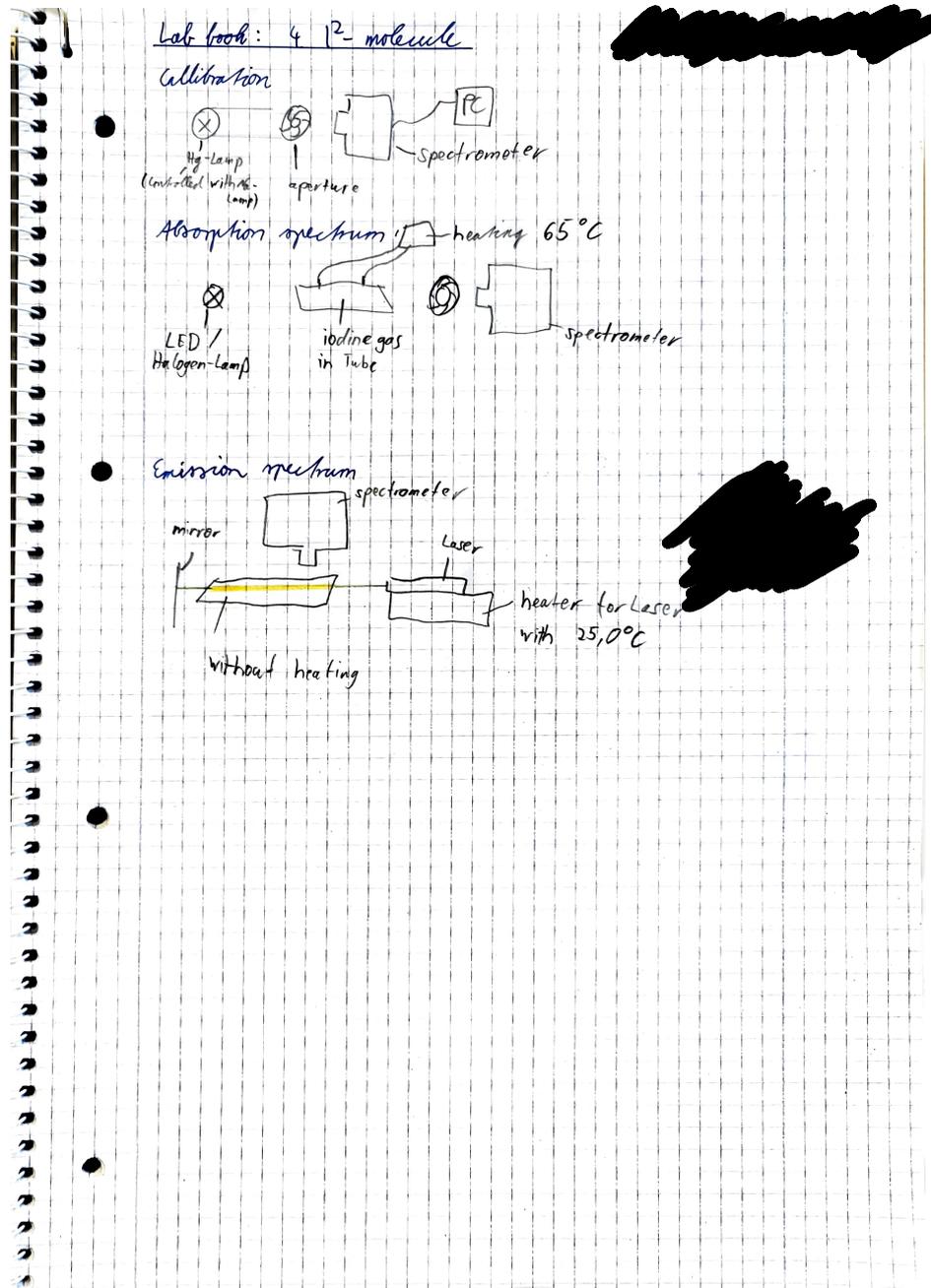


Figure 11: Lab book

literature

- [1] O. Optics, *Usb2000+ fiber optic spectrometer*, 2010.
- [2] LibreTexts. “Chem310l physical chemistry laboratory.” (Jan. 11, 2024), [Online]. Available: https://chem.libretexts.org/Courses/Duke_University/CHEM_310L%3A_Physical_Chemistry_I_Laboratory/CHEM310L_-_Physical_Chemistry_I_Lab_Manual/05%3A_Molecular_Spectroscopy_of_Iodine/5.04%3A_Part_I_-_Absorption_Spectrum_of_Iodine_Vapor_-_Experimental (visited on 09/12/2024).
- [3] S. B. Bayram and M. V. Freamat. “A spectral analysis of laser induced fluorescence of diatomic iodine.” (Aug. 25, 2015), [Online]. Available: https://www.researchgate.net/publication/279968251_A_Spectral_Analysis_of_Laser_Induced_Fluorescence_of_Iodine#read (visited on 09/12/2024).
- [4] Particle Data Group, S. Navas *et al.*, “Review of particle physics,” *Phys. Rev. D*, vol. 110, no. 3, p. 030001, 2024. DOI: [10.1103/PhysRevD.110.030001](https://doi.org/10.1103/PhysRevD.110.030001).
- [5] Thorlabs. “Cps532-c2 - collimated laser-diode-pumped dpss laser module, 532 nm, 0.9 mw, round beam, ø11 mm housing.” (), [Online]. Available: <https://www.thorlabs.com/thorproduct.cfm?partnumber=CPS532-C2> (visited on 09/12/2024).
- [6] N. I. of Standards and Technology. “Iodine.” (2023), [Online]. Available: <https://webbook.nist.gov/cgi/cbook.cgi?ID=C7553562&Mask=1000#Diatomic> (visited on 09/12/2024).